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Three-sublattice order in the SU(3) Heisenberg model

Bela Bauer (Station Q, Santa Barbara)
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Multi-Grid approach for matrix product states

Michele Dolfi & Matthias Troyer (ETH Zurich)
Bela Bauer (Station Q)

arXiv:1203.6363

Challenges for numerics

Fermionic lattice models

- Phase diagrams of even simple models such as the *t-J* or Hubbard model are still disputed

Realistic systems

- Materials, quantum chemistry
- Structure factors of quasi-*1d* frustrated magnets for neutron scattering
- Fraction Quantum Hall systems

Frustrated spin systems

- Existence of exotic phases, in particular without local order as $T \rightarrow 0$
- Topological spin liquids
- Gapless spin liquids: Fermi sea of fractionalized excitations
- *SU(N)* models, orbital models, Kondo models

Time evolution

- Equilibration/relaxation/thermalization
- Preparation of states in an optical lattice

Tensor networks in 2d

PEPS, MERA, EPS, TTN, ...

- Polynomial scaling for 2*d* systems, or even thermodynamic limit immediately
- Small bond dimension and little numerical experience

Elegant, but somewhat uncontrolled

The dark side: DMRG

- DMRG scales exponentially in 2*d*!
- System sizes much larger than ED
- Several recent successes

Brute force, but well-controlled

Maybe we should combine approaches?

Multi-flavor Hubbard models

- Multi-flavor Hubbard models can be realized in cold atomic gases

$$H = -t \sum_{\langle i,j \rangle} \sum_{\alpha} \left(c^\dagger_{i\alpha} c_{j\alpha} + \mathrm{h.c.} \right) + U \sum_i \sum_{\alpha \neq \beta} n_{i\alpha} n_{i\beta}$$

- Lots of cooling and commensurable filling: ***Mott insulator***
- Even more cooling: ***spin order***

SU(2)

- Square lattice: antiferromagnet
- Triangular lattice: 120° order

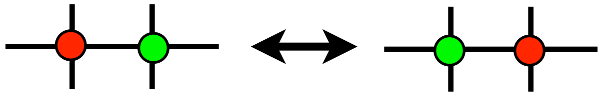
SU(3)

- Fix one particle per site
- Spin order unknown for both triangular and square lattice

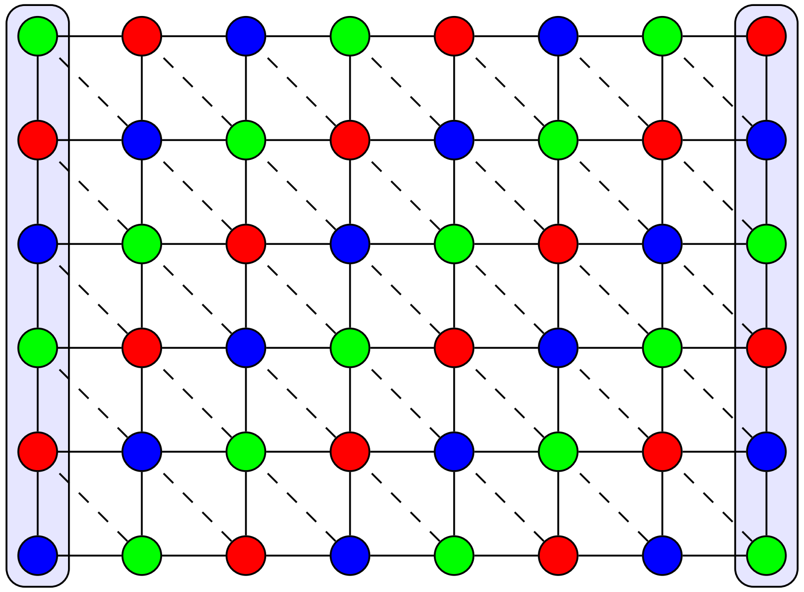
SU(3) Heisenberg model

- We concentrate on three-flavor case with one particle per site and derive an effective model in *t/U*

$$H = J \sum_{\langle i,j \rangle} \sum_{\alpha,\beta} |\alpha_i \beta_j\rangle\langle \beta_i \alpha_j|$$

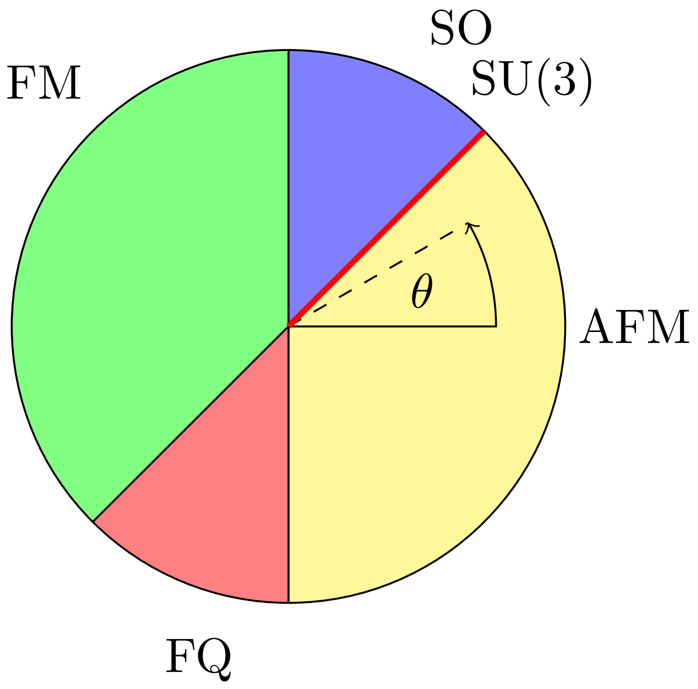


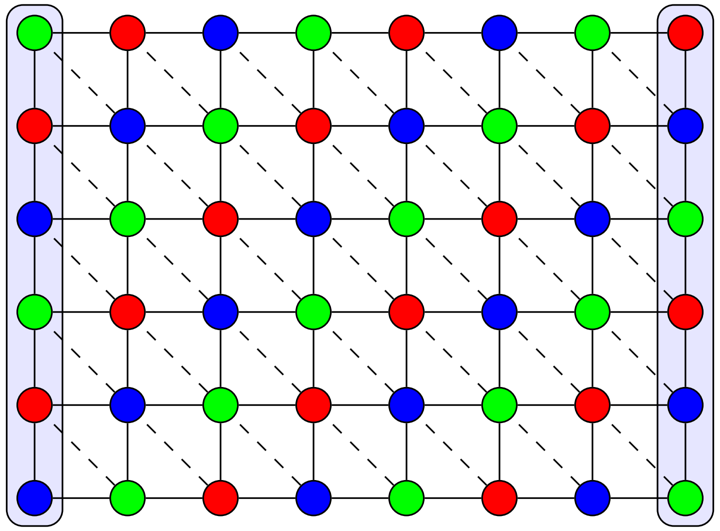
- We study the **square** and **triangular** lattice



Spin-1 bilinear-biquadratic model

$$H = \sum_{\langle i,j \rangle} \left[\cos\theta (\vec{S}_i \cdot \vec{S}_j) + \sin\theta (\vec{S}_i \cdot \vec{S}_j)^2 \right]$$





- Mean-field phase diagram for the **square lattice** (Papanicolaou, 1988):
  - SU(3) point at transition from antiferromagnet to "semi-ordered phase"
  - Square lattice does not give enough constraints to uniquely fix ordering in that phase
- **Triangular lattice**:
  - Enough constraints at the SU(3) point: **three-sublattice order**

Mean-field phases

Square lattice

- Semi-ordered phase is characterized by infinitely many degenerate ground states between 2- and 3-sublattice order

→

Do quantum fluctuations select some type of order, or does a completely different phase emerge?

Previous work: Tóth et al, PRL 2010

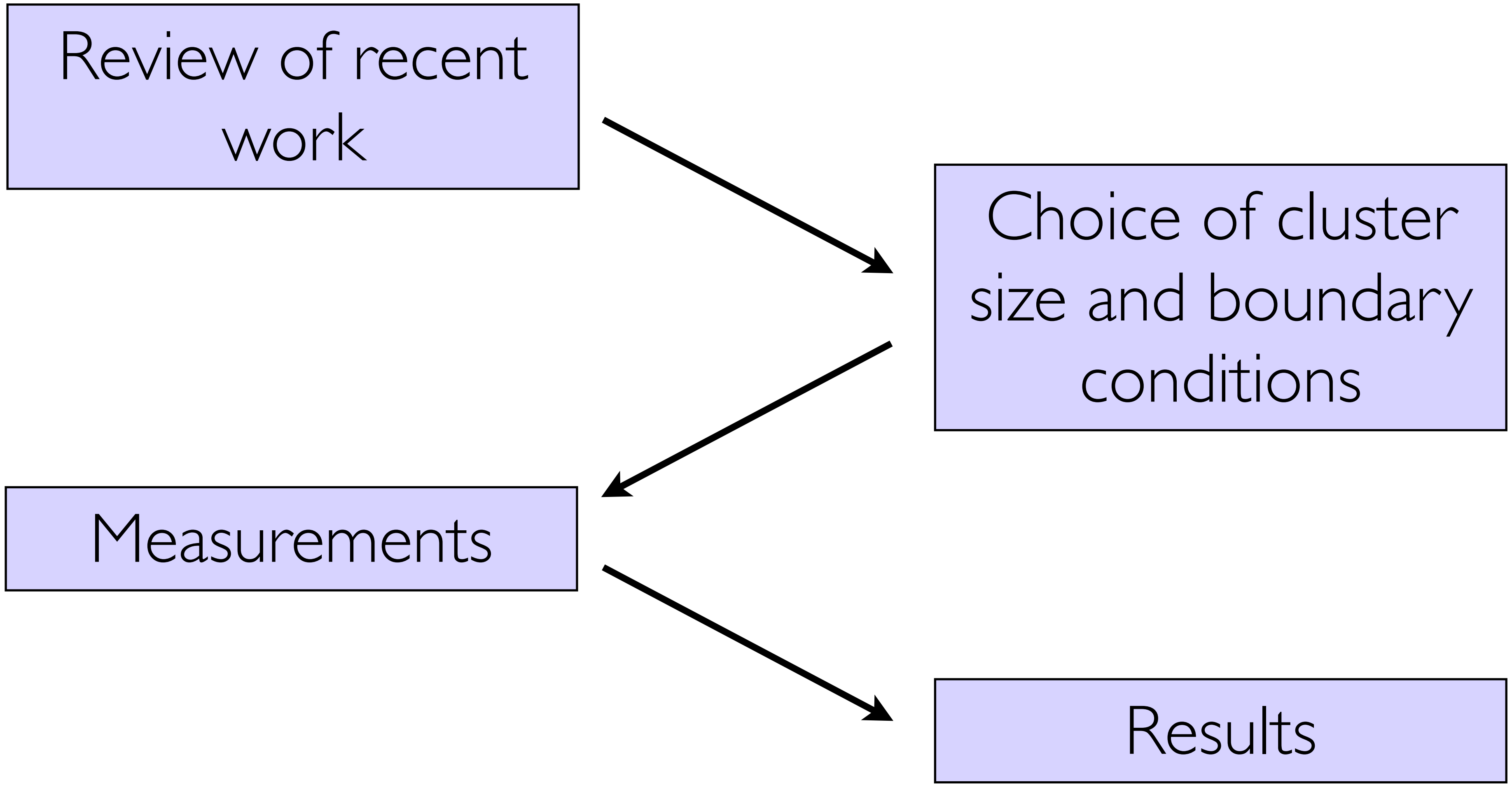
Triangular lattice

- SU(3) point has three-sublattice order

→

Is this stable under quantum fluctuations?

The dark side: DMRG in 2*d*



Review of recent work

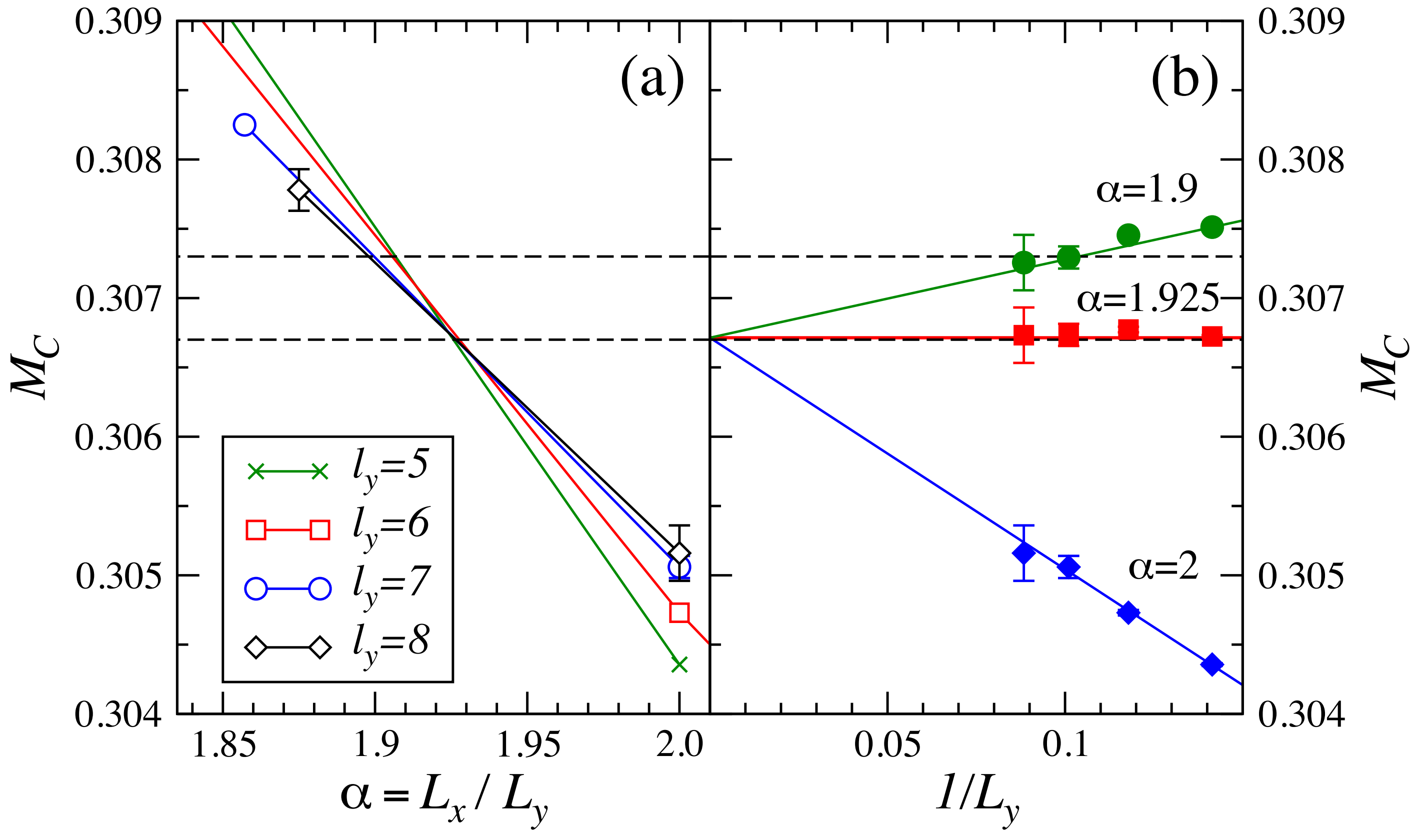
Choice of cluster size and boundary conditions

Measurements

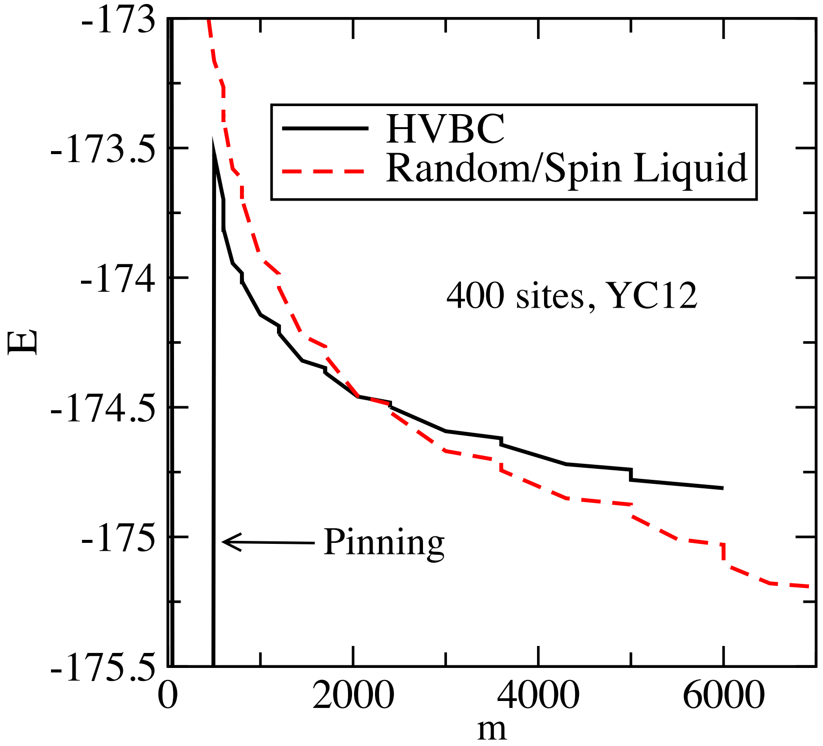
Results

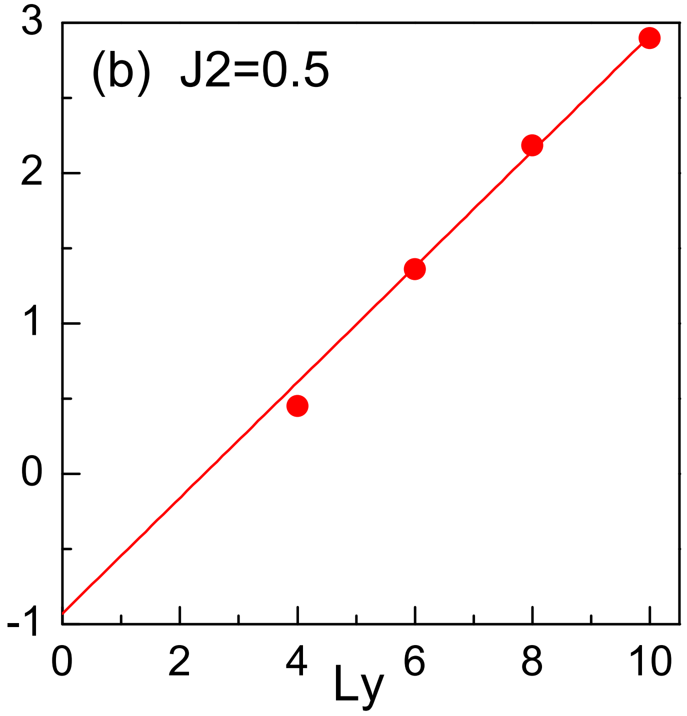
Some recent 2*d* DMRG results

- *White & Chernyshev, PRL 99, 127004 (2007)*
  - SU(2) Heisenberg model on square and triangular lattice
  - Results for square lattice with similar accuracy as MC after careful extrapolation in truncated weight and system size
  - Lots of prior knowledge from spin-wave theory



Some recent 2*d* DMRG results



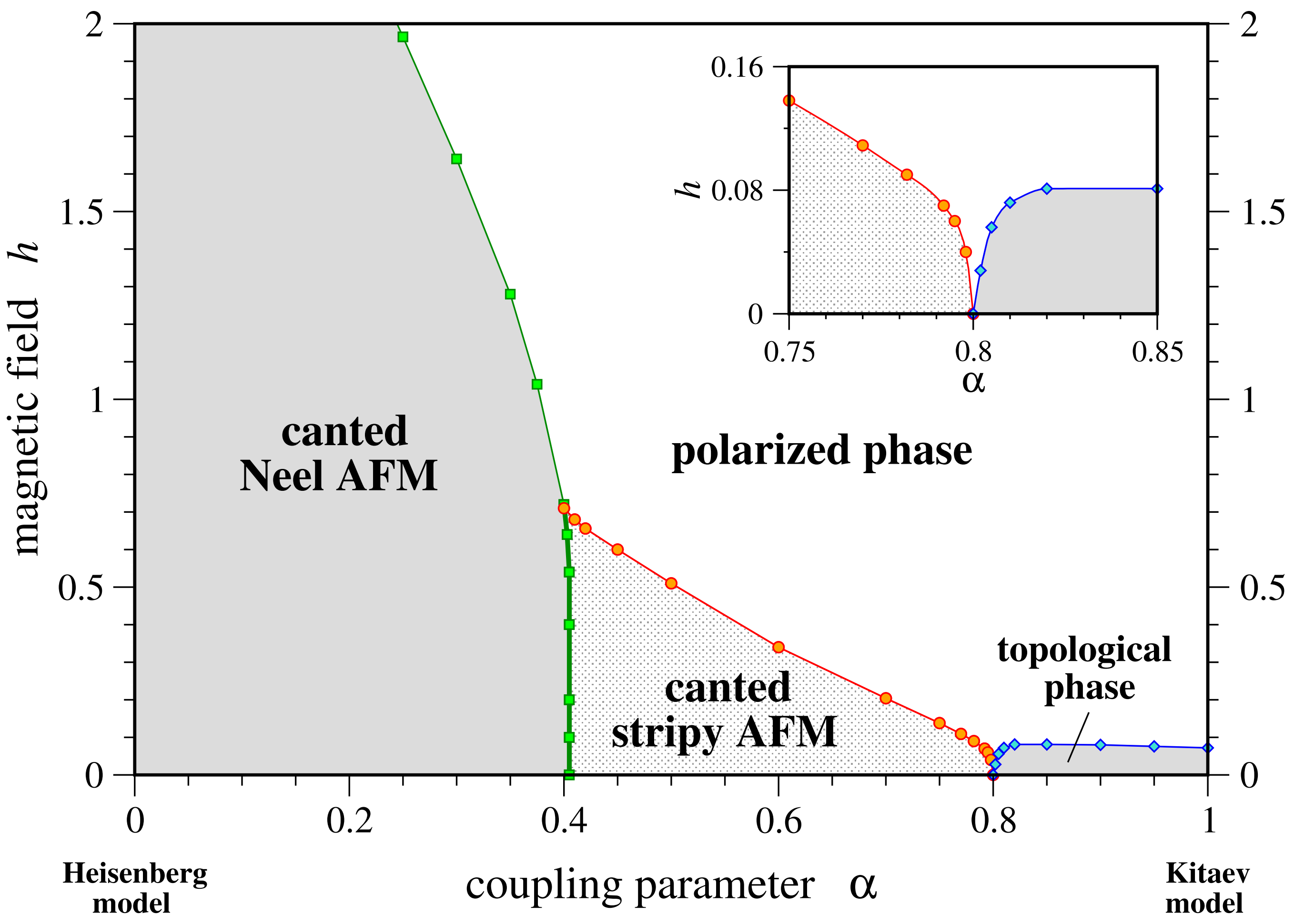


- *Yan, Huse & White, Science 332, 6034 (2011)*
  - Spin liquid ground state on the Kagome lattice
  - Previous best energy: *Evenbly & Vidal, PRL 104, 187203 (2010)*
  - See also Stefan Depenbrock's poster downstairs

- *Jiang, Yao & Balents 2011, arXiv:1112.2241*
  - Spin liquid ground state in the J_1-J_2 model on the square lattice
  - Previous work with PEPS: *Murg, Verstraete & Cirac, PRB 79, 195119 (2009)*
  - Current work with PEPS: *Wang, Gu, Verstraete & Wen, arXiv:1112.3331*

Some recent 2*d* DMRG results

- *Jiang, Gu, Qi & Trebst, PRB 83, 245104 (2011)*
  - Heisenberg-Kitaev model with magnetic field
  - Interpolates between Kitaev's honeycomb model and Heisenberg model and describes certain Iridate compounds



The dark side: DMRG in 2*d*

👍 Review of recent work

Choice of cluster size and boundary conditions

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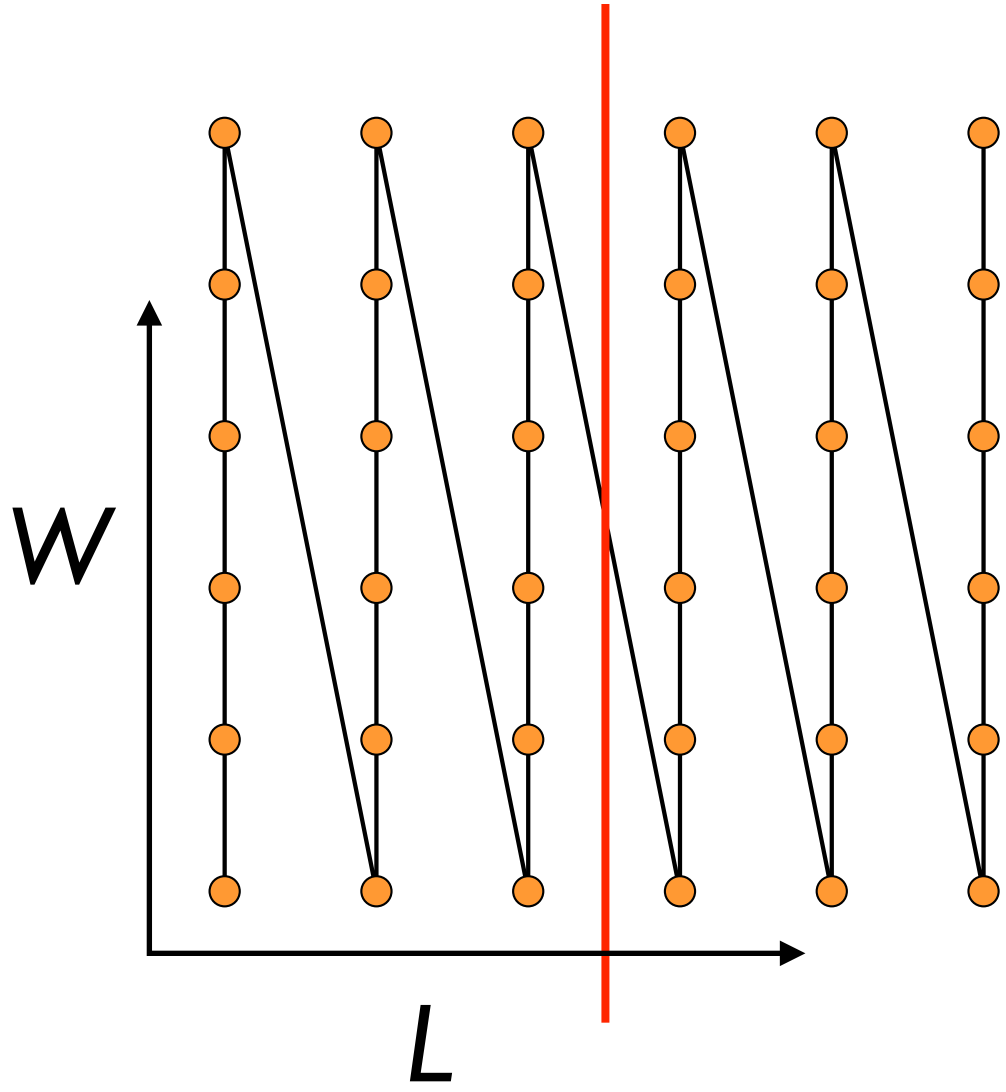
DMRG in 2*d*: entanglement



- Bond dimension of the MPS:

$$M \sim \exp S$$

- Scaling of entanglement:

$$S \sim W$$

$$\cancel{S \sim L}$$

- *There is an easy (L) and a hard (W) direction!*

Use long rectangles!

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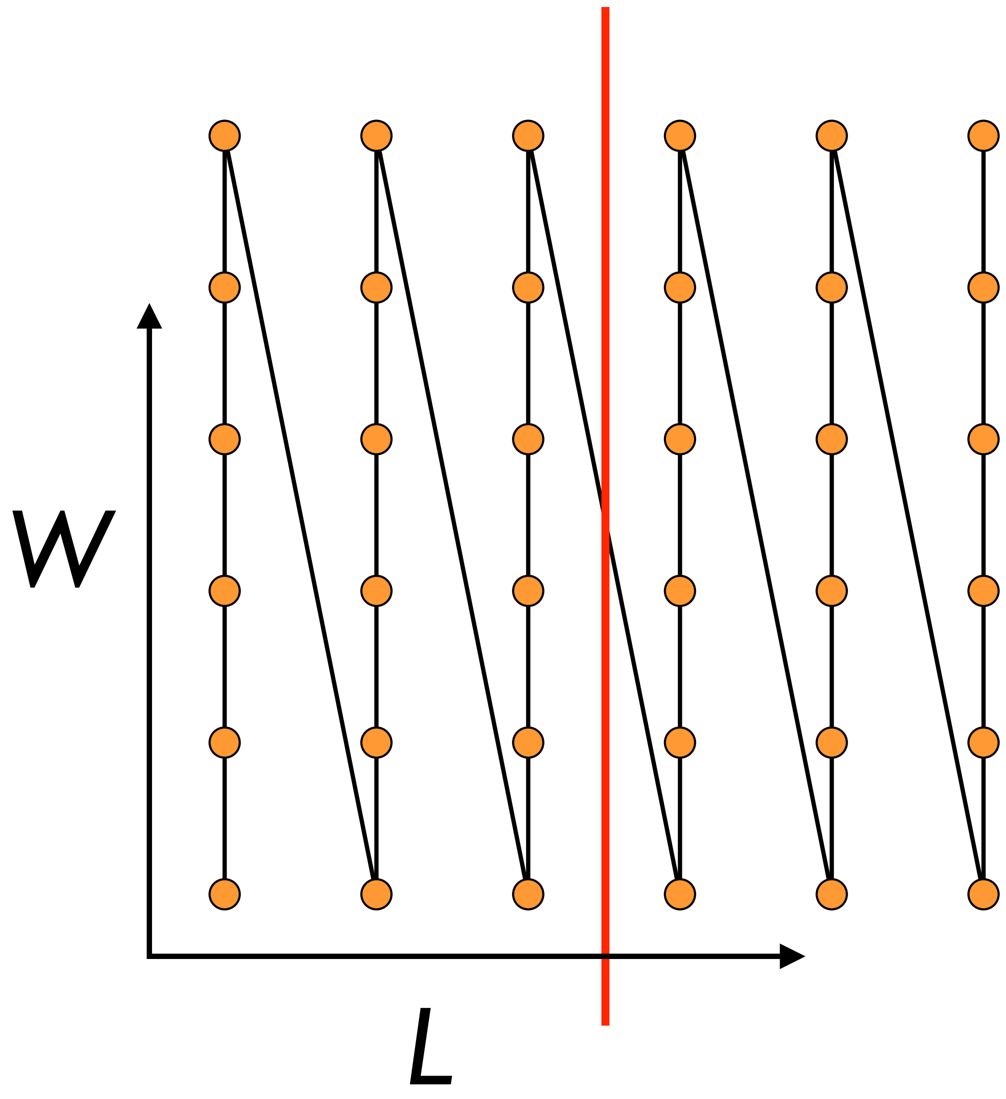
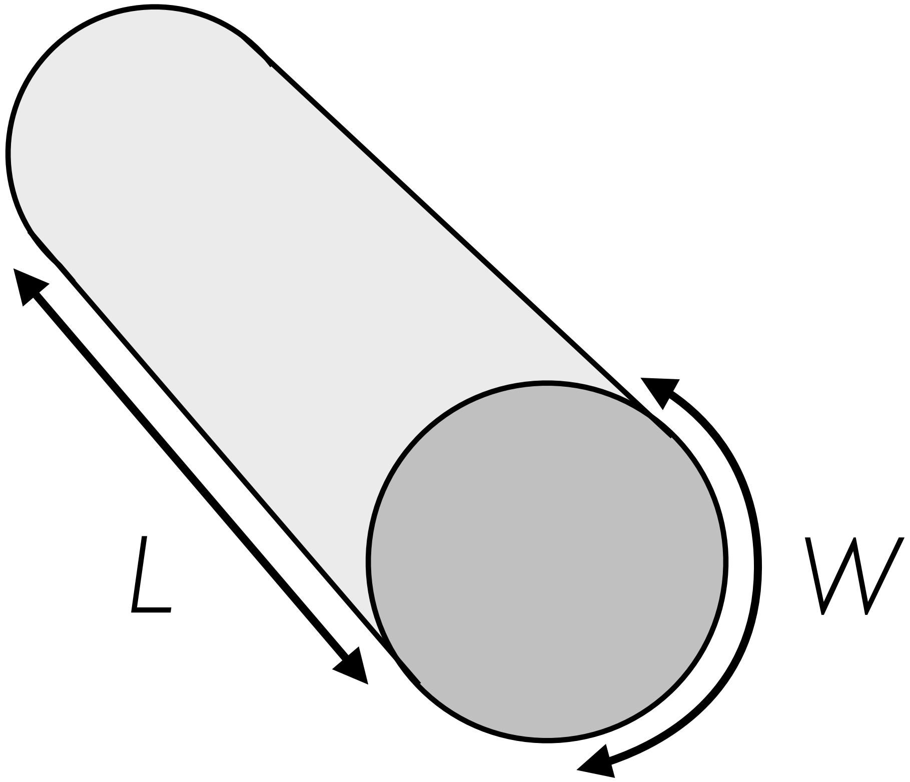
DMRG in 2*d*: boundaries



- Physically, periodic boundary conditions are often preferable
- In 1*d* DMRG: $S \rightarrow 2S$
  - Naive approaches need the square of the bond dimension, better approaches exist but numerically not as robust and precise
- PBC in 2*d* DMRG:
  - *L* direction: same problem as 1*d*
  - *W* direction: not as bad

DMRG in 2*d*: boundaries



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  - *W* direction: not as bad

Use cylinders, avoid the torus!

Scaling

MPO bond dimension: $D \sim W$

Computation: $\mathcal{O}(LW \cdot D \cdot M^3) + \mathcal{O}(LW \cdot D^2 \cdot M^2)$

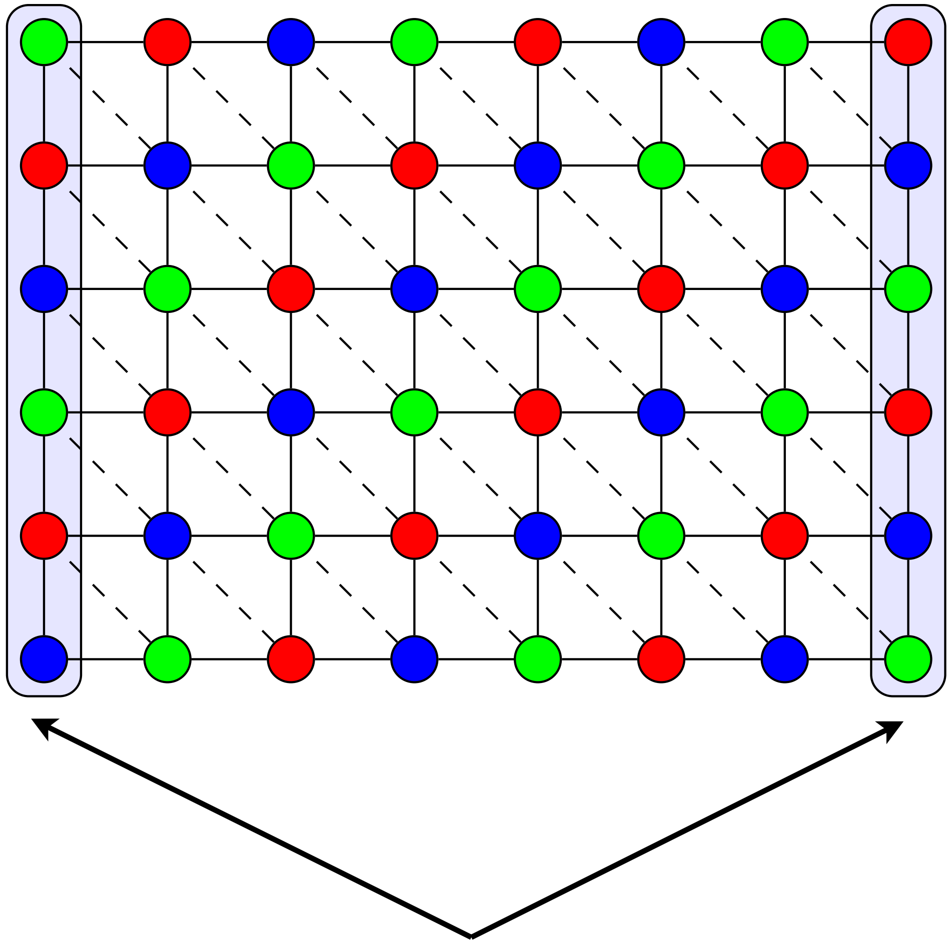
Memory: $\mathcal{O}(D \cdot M^2)$

Disk: $\mathcal{O}(LW \cdot D \cdot M^2)$

↓

Without *SU(2)* symmetry: memory and disk space are limiting factors!

DMRG in 2*d*: local moments



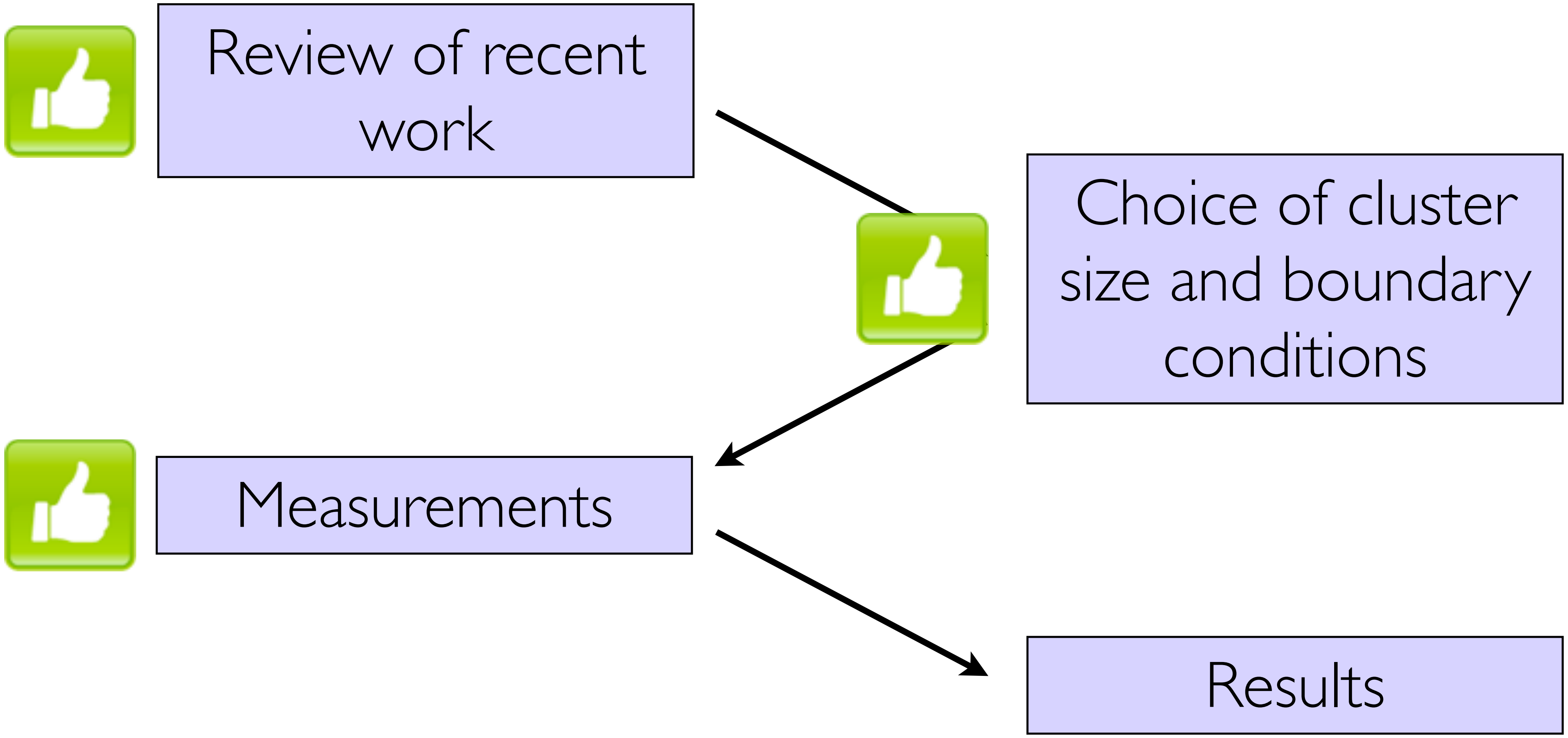
"Pinned" order with flavor-dependent chemical potential

- Long-range correlations are not reliable for 2d systems
- Break symmetries by hand at the boundary and watch the system far away!
- Reduces entanglement significantly

DMRG in 2*d*: extrapolation

- Long-standing question: ***what's the correct way to extrapolate?***
  - ***Number of states***: usually not very reliable
  - ***Truncated weight***: standard technique, but sometimes difficult with single-site update
  - ***Energy variance***: computationally difficult for large 2*d* system and complex Hamiltonians

The dark side: DMRG in 2*d*



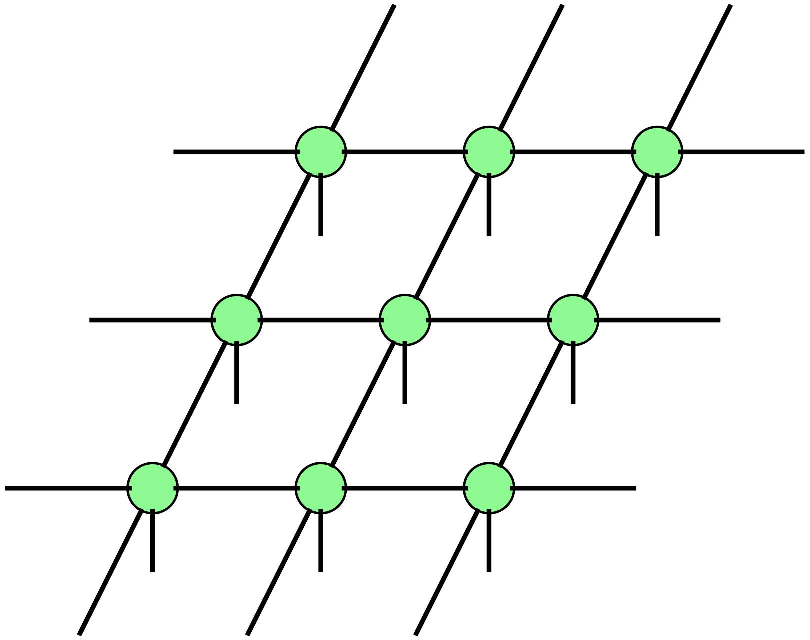
👍 Review of recent work

👍 Choice of cluster size and boundary conditions

👍 Measurements

Results

iPEPS



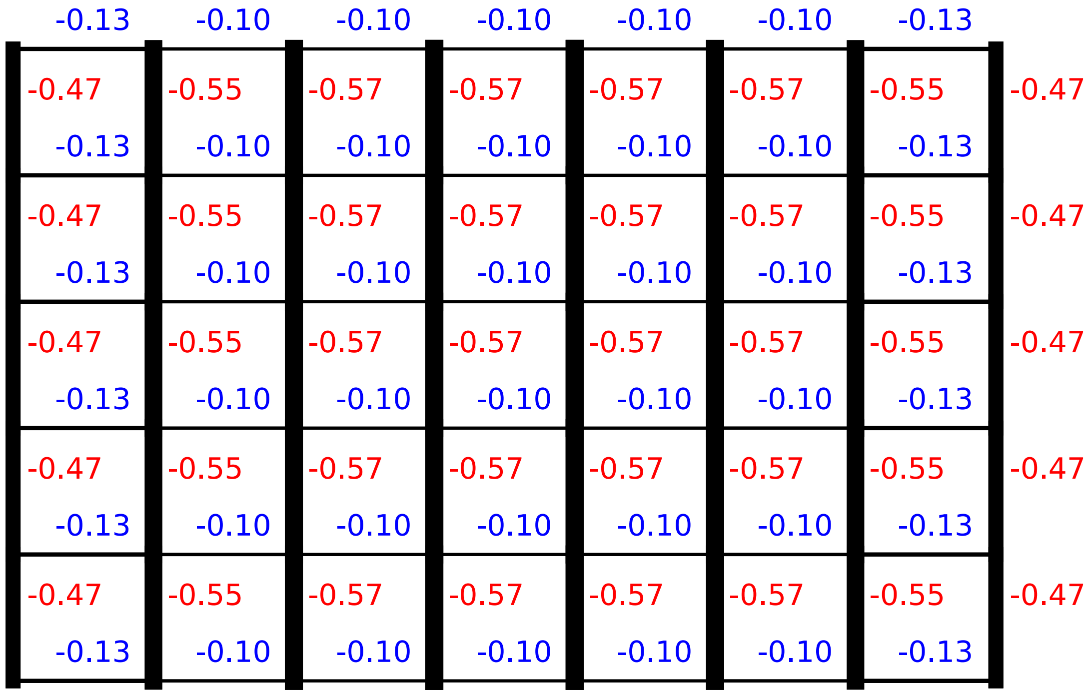
- Square lattice ansatz for both square and triangular lattice: *P. Corboz et al, PRB 82, 45119 (2010)*
- Directional corner transfer matrix scheme for general unit cells: *P. Corboz et al, PRB 84, 041108 (2011)*
  - *3x3* unit cell to stabilize three-sublattice state, *2x2* unit cell for antiferromagnet
- Z_3 symmetry: *Bauer et al, PRB 83, 125106 (2011)*

DMRG results

- Unknown finite-size scaling: stick to (almost) square systems
- Computational challenges:
  - Large dimension of the MPO (~twice of *SU(2)* case)
  - Need to use large bond dimension already in early stages due to non-mean field nature of the order
  - Very large entanglement
- Up to $M \sim 5000$ states, check for up to $M \sim 6400$ in some cases → system size up to *8x8*

DMRG results

6x8 square lattice,
cylindrical BCs,
M=4800



-0.13 -0.10 -0.10 -0.10 -0.10 -0.10 -0.13
-0.47 -0.55 -0.57 -0.57 -0.57 -0.57 -0.55 -0.47
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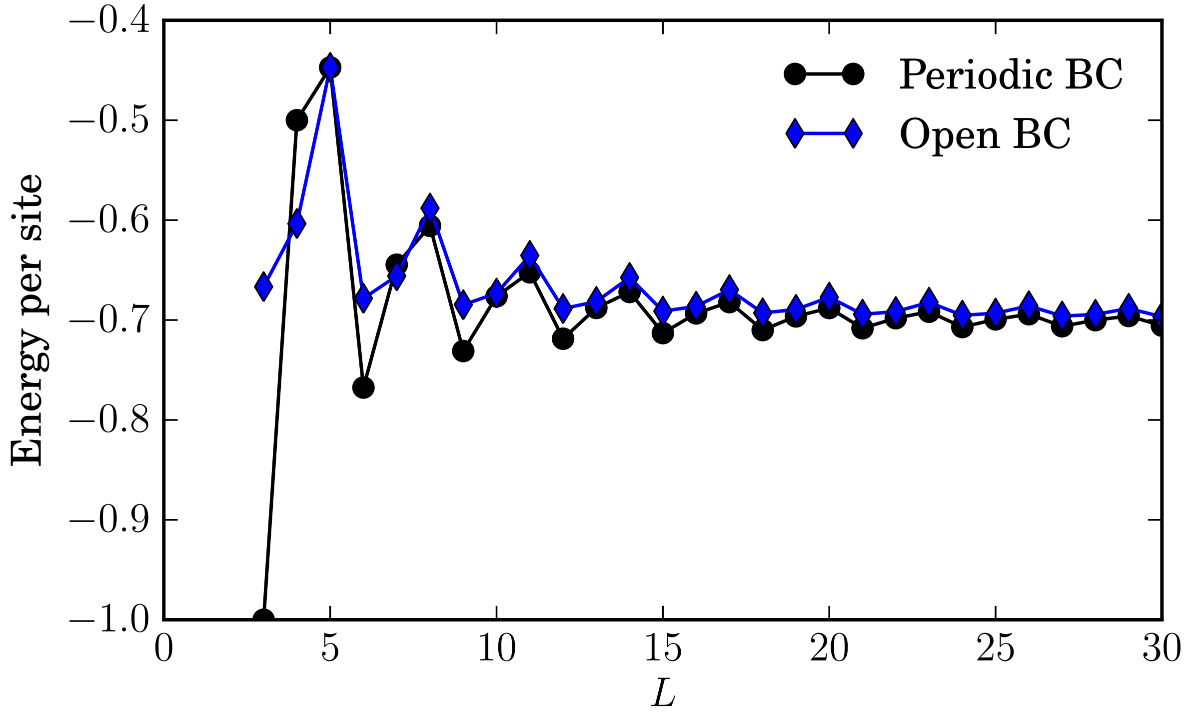
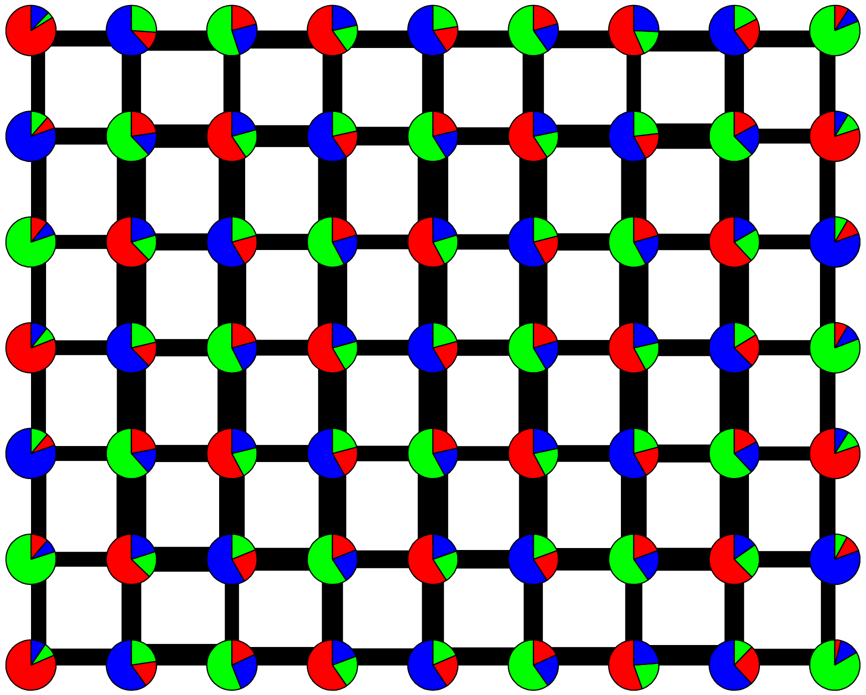
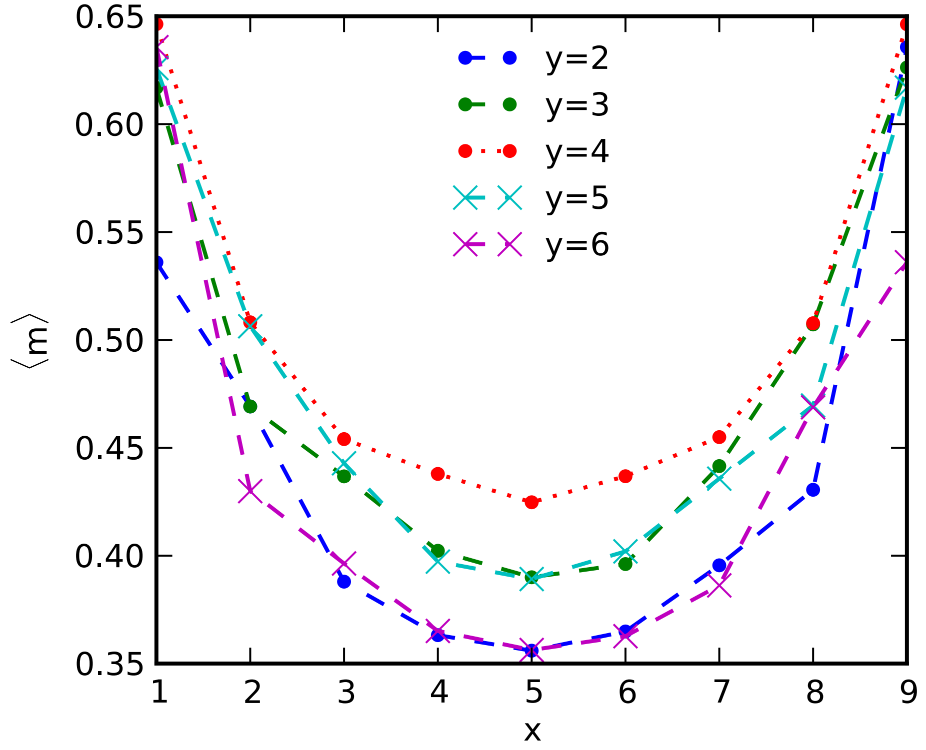
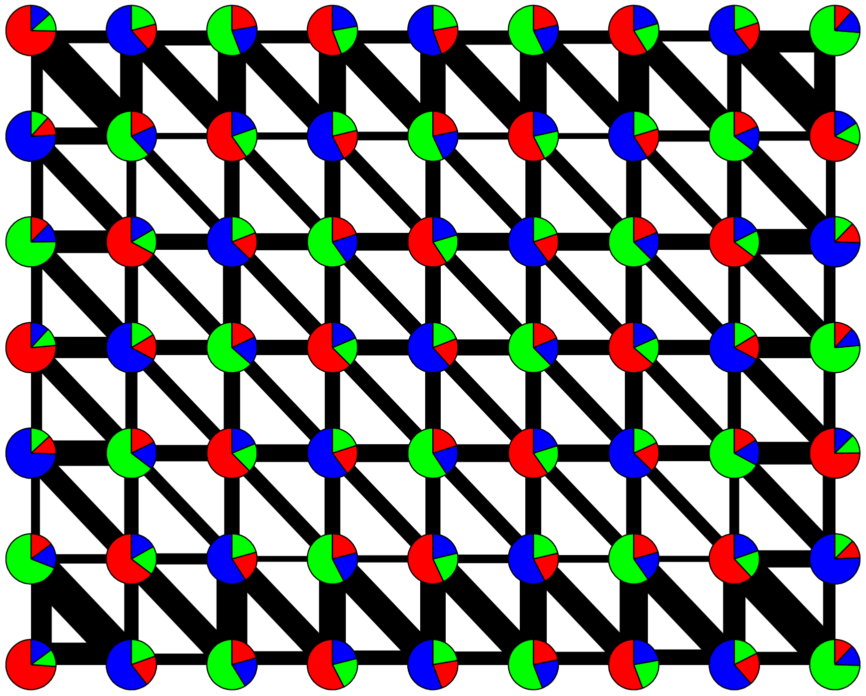


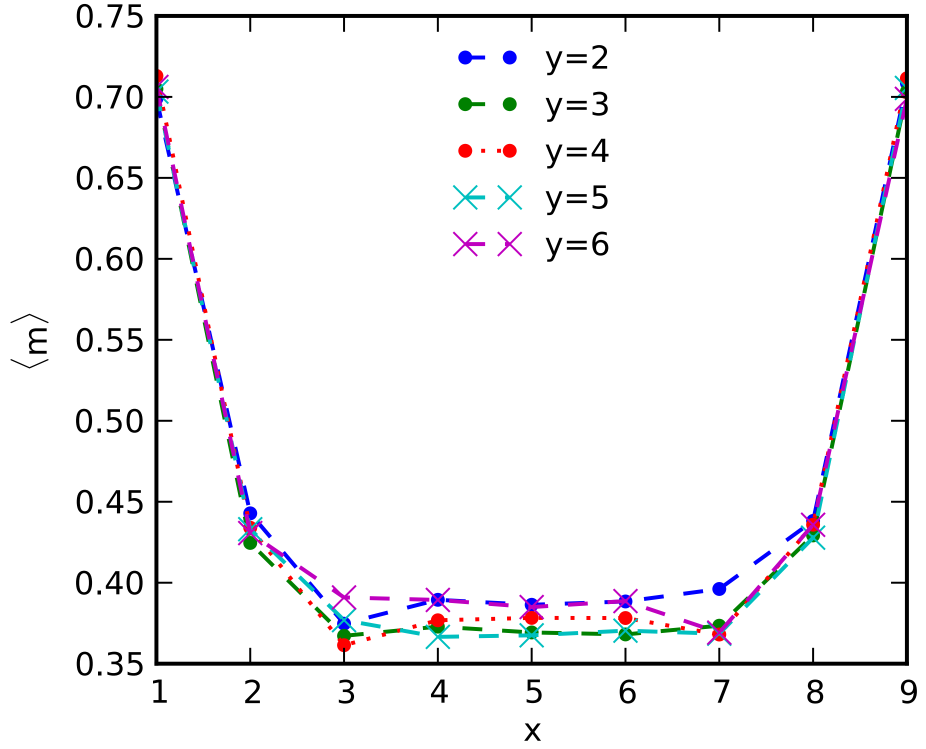
Huge finite-size corrections for periodic chain → use open boundaries after all

DMRG results









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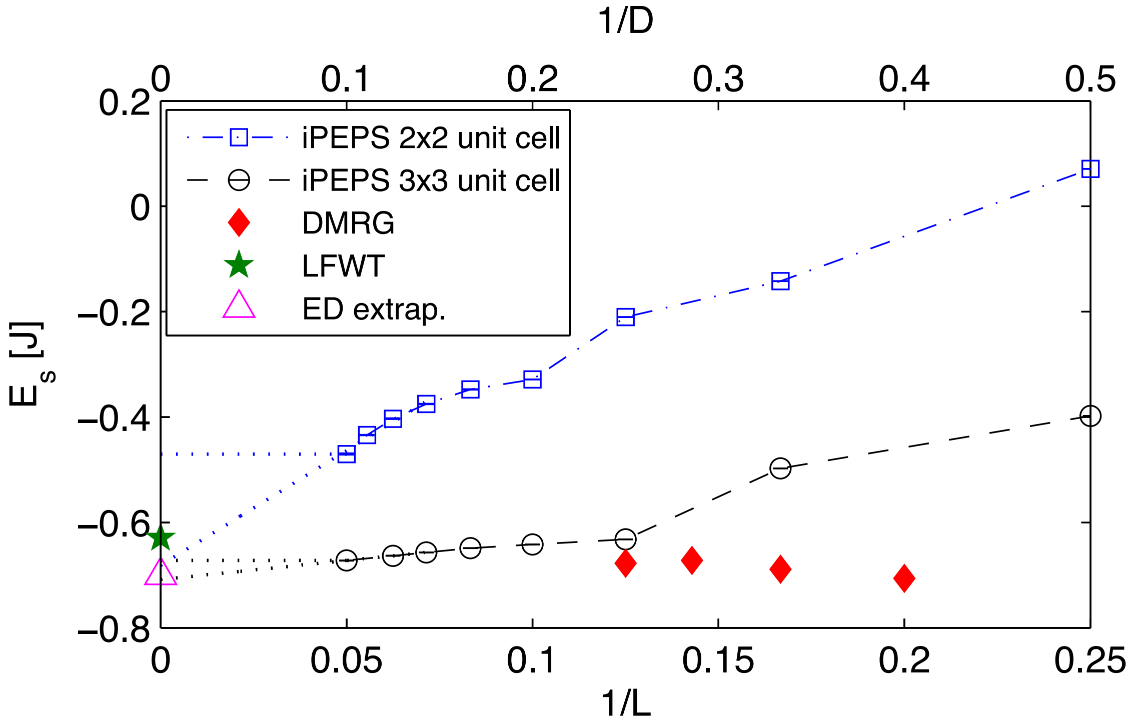
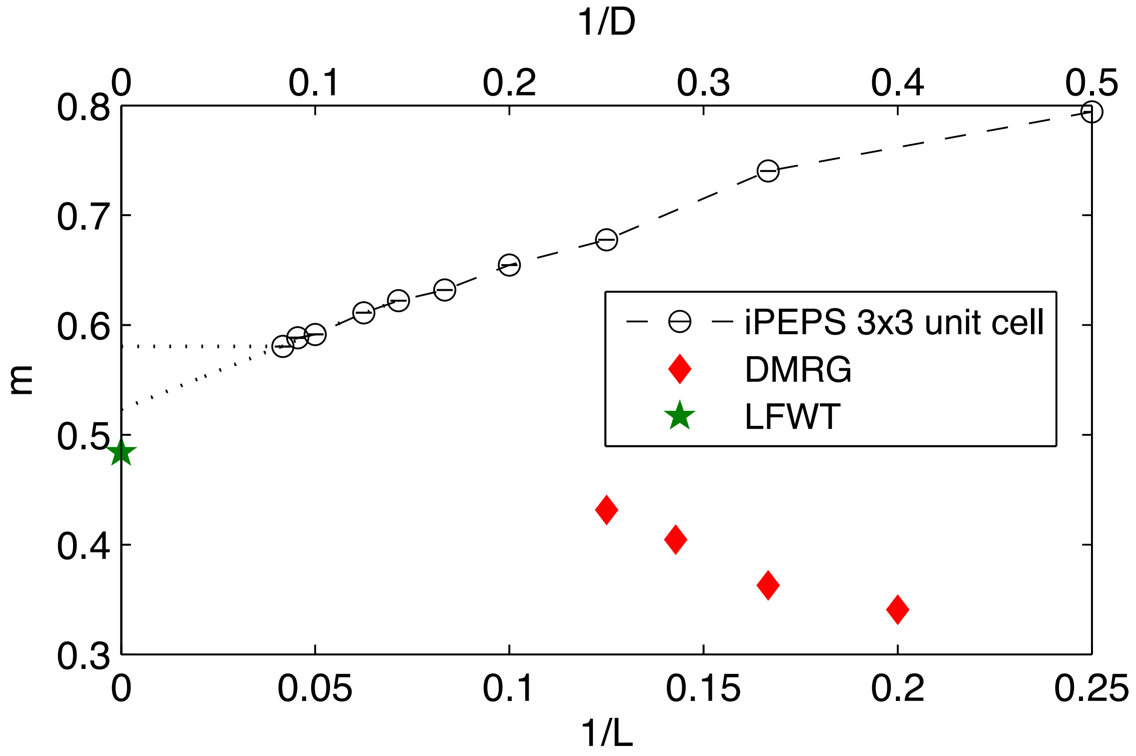
Triangular lattice

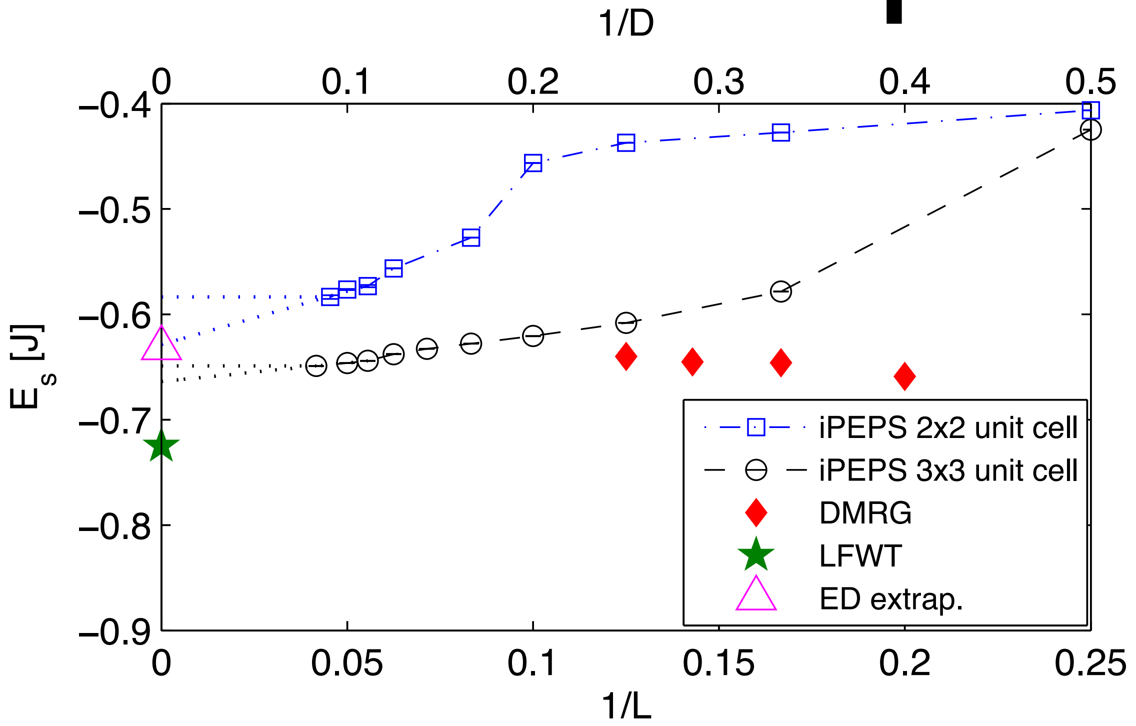


- Energies of all methods match qualitatively
- iPEPS 3x3 is much lower than iPEPS 2x2
- DMRG has weak finite-size dependence

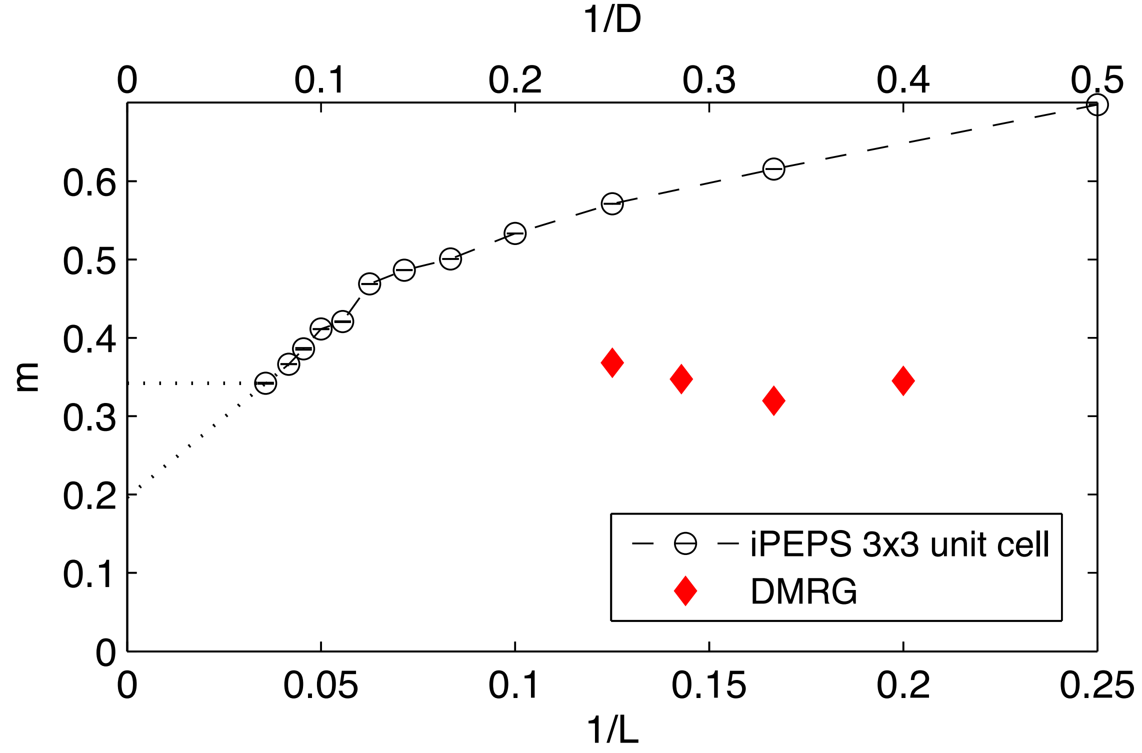


- Order parameters are consistent with 40-50 % of saturation moment

Square lattice



- Again, iPEPS 3x3 has much lower energy than iPEPS 2x2
- DMRG energies are comparable and consistent with ED



- Strong dependence of moment in iPEPS calculation leaves a large margin of error
- DMRG results seem consistent with magnetization in the range 30-40 % of the saturation moment

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Multi-Grid approach for matrix product states

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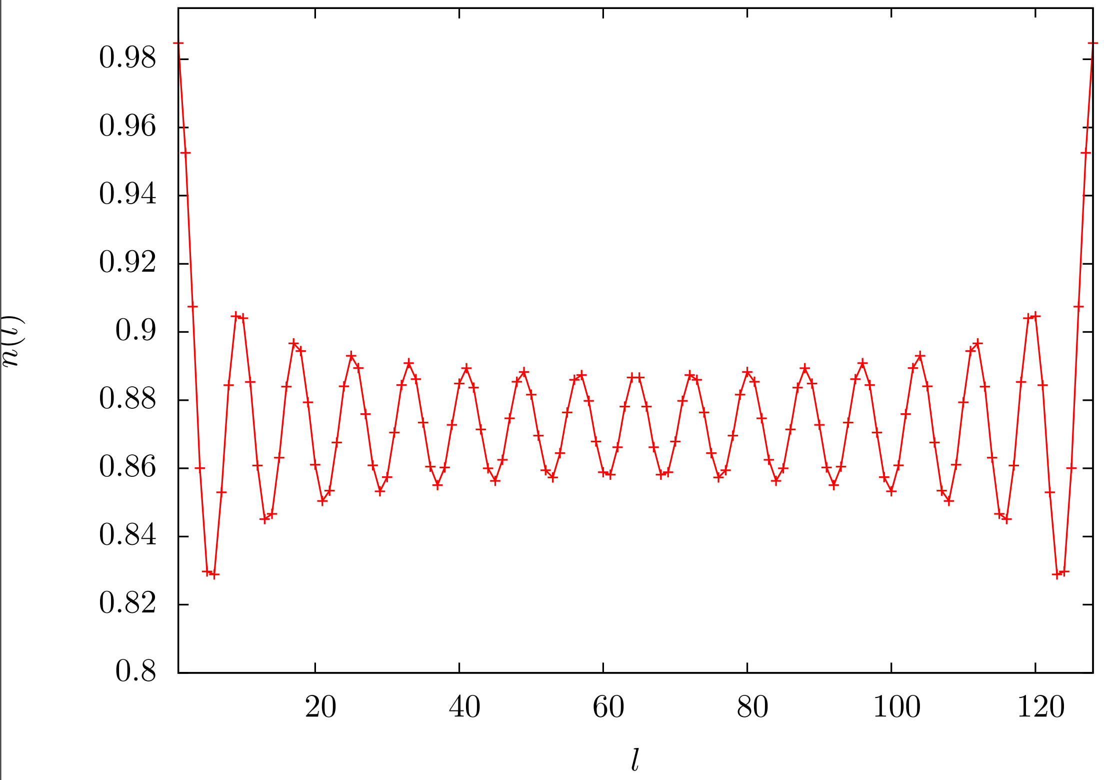
Systems with various scales

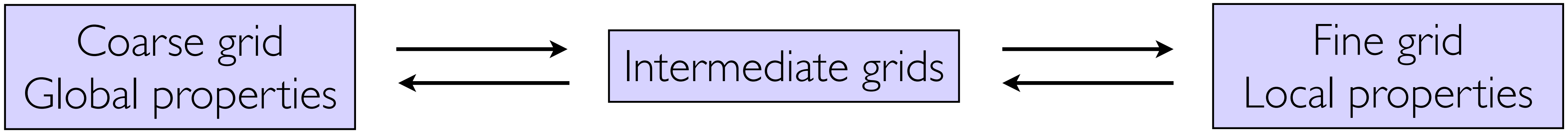
Example: doped Hubbard ladder



- Local optimization (DMRG) ***almost*** always works
- One class of exceptions: ***dilute systems***
    - Weakly doped systems (*cf.* Davide Rossini's talk last Monday)
    - Discretized continuous systems
- These systems have various length scales:
    - Doped systems: lattice spacing, size of a hole, global density modulation
    - Discretized continuous systems: discretization dx, external potential
- Energy scales: hopping ~ $1/dx^2$, interaction ~ $1/dx$, potential ~ 1

Multi-grid approaches

- Standard method for partial differential equations: solve the system on different length scales

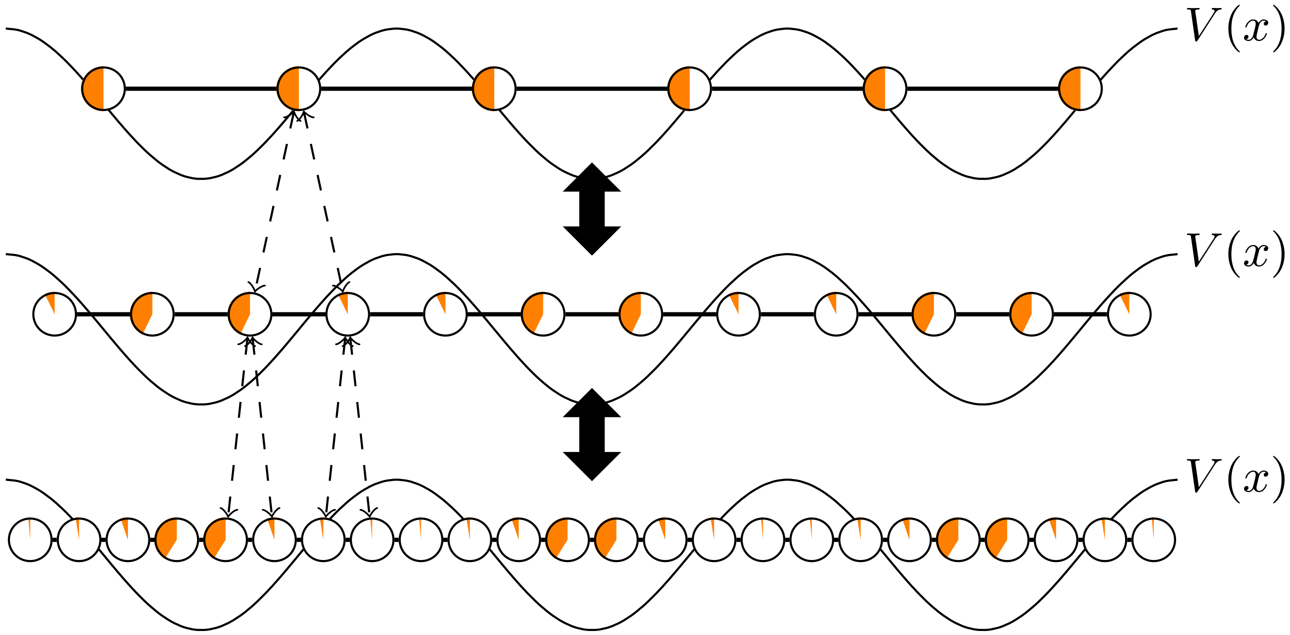


Coarse grid
Global properties

Intermediate grids

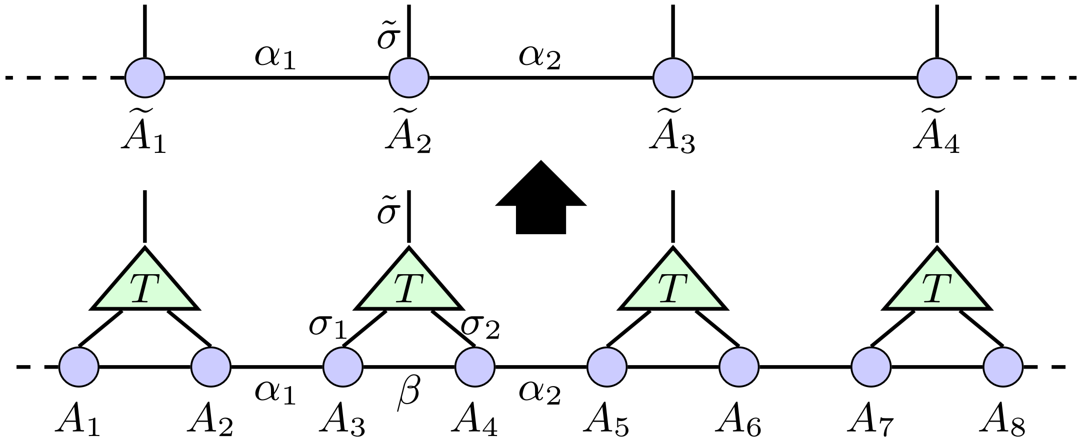
Fine grid
Local properties

- Example: bosons with contact interaction in a shallow optical lattice

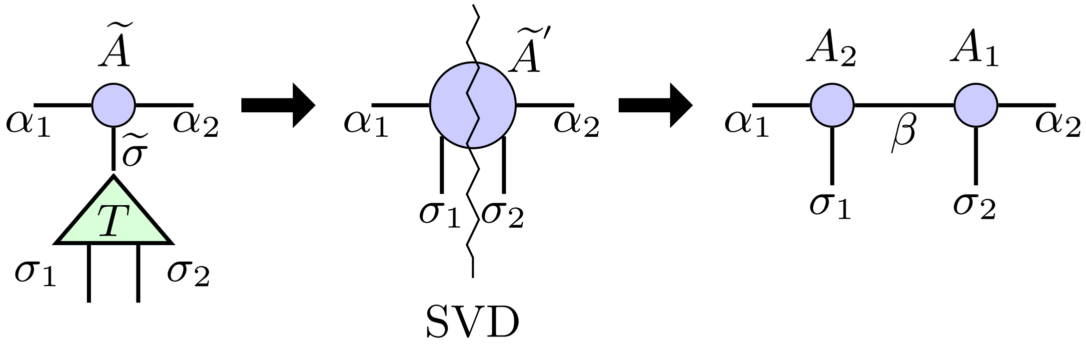


Multi-grid & MPS

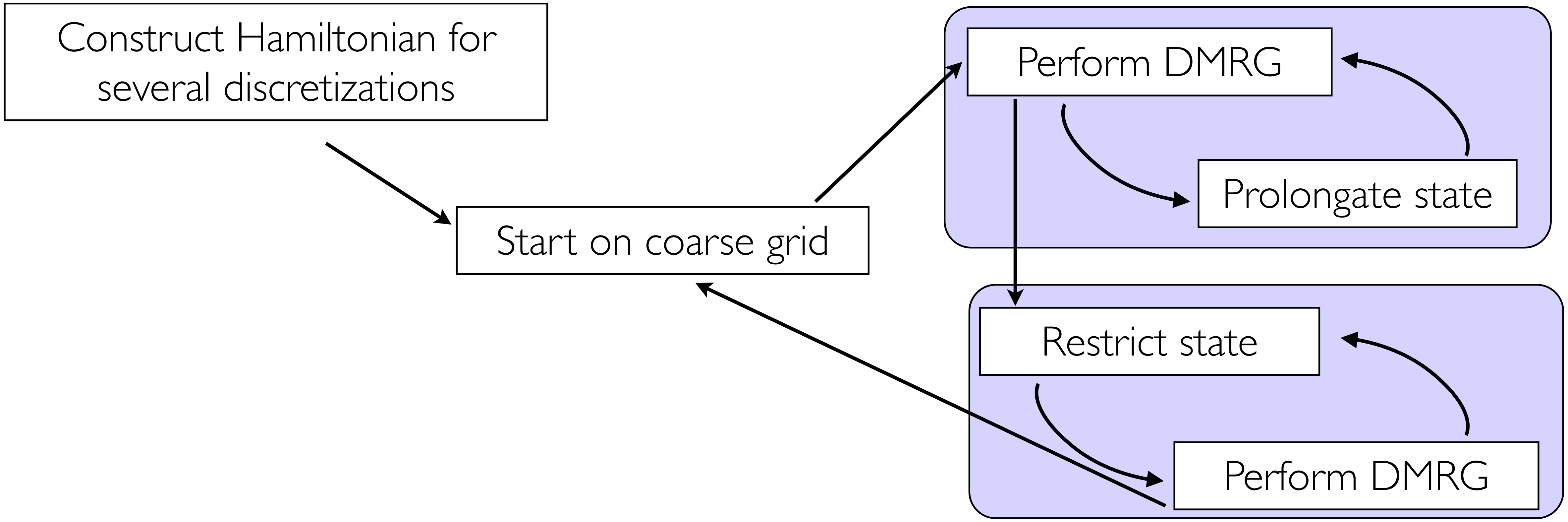
Restriction:



Prolongation:



Multi-grid & MPS



Construct Hamiltonian for several discretizations

Start on coarse grid

Perform DMRG

Prolongate state

Restrict state

Perform DMRG

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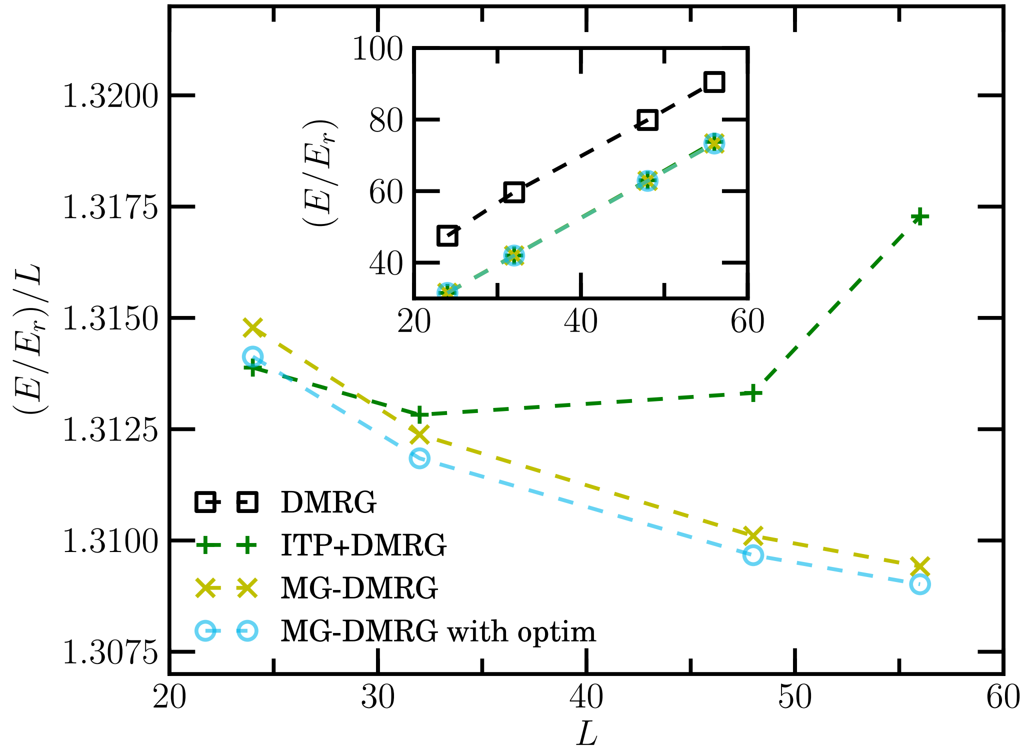
MG-DMRG: results



- Convergence often much more reliable than standard DMRG approaches
- Key difference to tree tensor network: ***the final result is only an MPS on one layer***
- Extension to lattice models: how to construct Hamiltonians for coarser lattice?
  - CORE? Applying isometries to the MPO?

Conclusion

- Convincing numerical evidence for three-sublattice order on both the square and the triangular lattice
- **Completely different ordering mechanisms:**
    - Unique order at mean-field level on triangular lattice
    - Quantum fluctuations select the three-sublattice order over other states on the square lattice
- **Combination of two tensor-network states builds more trust in results**
- **Both iPEPS and 2d DMRG are valuable tools for understanding 2d systems**

- **MG-DMRG provides a way to converge MPS ground states reliably when system has various length scales**